

Metallicity and its low-temperature behavior in dilute two-dimensional carrier systems

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We theoretically consider the temperature-dependent and density dependent transport properties of semiconductor-based two-dimensional (2D) carrier systems within the RPA-Boltzmann (RPA, random-phase approximation) transport theory, taking into account realistic screened charged impurity scattering in the semiconductor. We derive a leading behavior in the transport property, which is exact in the strict 2D approximation and provides a zeroth-order explanation for the strength of metallicity in various 2D carrier systems. By carefully comparing the calculated full nonlinear temperature dependence of electronic resistivity at low temperatures with the corresponding asymptotic analytic form obtained in the $T/T_F \rightarrow 0$ limit, both within the RPA screened charged impurity scattering theory, we critically discuss the applicability of the linear temperature-dependent correction to the low-temperature resistivity in 2D semiconductor structures. We find quite generally that for charged ionized impurity scattering screened by the electronic dielectric function (within RPA or its suitable generalizations including local-field corrections), the resistivity obeys the asymptotic linear form only in the extreme low-temperature limit of $T/T_F \leq 0.05$. We point out the experimental implications of our findings and discuss in the context of the screening theory the relative strengths of metallicity in different 2D systems.

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I. INTRODUCTION

A great deal of attention has recently been focused on the temperature dependence of carrier [both electrons and holes, depending on whether the two-dimensional (2D) system is n doped or p doped—in this paper the terminology “electron” or “electronic” generically refers to electrons or holes depending on the 2D system being considered] resistivity $\rho(T)$ at low temperatures (and densities), following the pioneering experimental report by Kravchenko and collaborators¹ that the measured low temperature $\rho(T)$ shows very strong “metallic” temperature dependence [i.e., $\rho(T)$ increasing with T] at some intermediate densities (the so-called metallic or the 2D “metal” phase) eventually making a transition to a strongly insulating state at low carrier densities (n). [At high electron densities $\rho(T)$ shows weak temperature dependence² similar to 3D metals.] In particular, $\rho(T)$ could increase by as much as a factor of 3 in 2D Si metal-oxide-semiconductor field-effect transistor (MOSFET’s) (for $n \sim 10^{11} \text{ cm}^{-2}$) as temperature changes from 50 mK to a few kelvin.^{1,3} While this metallicity [in this paper “metallicity” or “metallic behavior” will exclusively signify the unusually strong T dependence of $\rho(T)$ in the metallic phase above the critical density at which the system makes a transition to the manifestly insulating phase] is by far the strongest in n -Si MOSFET 2D structures, the phenomenon has by now been observed (with large quantitative variations in the strength of the metallicity) in essentially all the existing low density 2D semiconductor systems^{4–11} such as p -GaAs, p - and n -SiGe, Si on sapphire (SOS), n -GaAs, n -AlAs, etc. Our work [we concentrate here on n -Si metal-oxide-semiconductor (MOS), p -GaAs, and n -GaAs, as representative 2D systems] presented in this paper deals with the currently controversial issue of understanding this metallicity from a theoretical perspective. In particular, we use a conventional Fermi-liquid theory approach in explaining the strong temperature depen-

dence of $\rho(T)$ in the metallic phase. We use the well-established RPA-Boltzmann transport theory for calculating $\rho(T)$ for 2D carrier systems, taking into account resistive scattering of the carriers by RPA-screened charged impurity random potential. The basic physical picture is that of a strongly temperature-dependent effective disorder seen by the 2D electrons at low carrier densities due to the temperature-dependent screening of charged impurity scattering which gives rise to the dominant resistive mechanism in semiconductors at low temperatures. We have earlier obtained qualitative agreement with experimental low density $\rho(T)$ measured in Si-MOS,¹² p -GaAs,¹³ SiGe,¹⁴ Si-MOS with substrate bias,¹⁵ and n -GaAs 2D structures¹⁶ using this microscopic screening theory approach. For higher carrier densities, however, this screening theory is known¹⁸ to provide an excellent quantitative description of 2D carrier transport.

In this paper we consider, motivated by recent theoretical and experimental development, the leading-order temperature dependence of the 2D metallic resistivity in the low temperature, $T/T_F \rightarrow 0$, limit (where $T_F = E_F/k_B \propto n$ is the 2D Fermi temperature), and provide a qualitative explanation for the relative strength of metallicity in various 2D systems. Such a unifying qualitative explanation for the relative metallicity strengths in different materials has so far been lacking in the literature. The 2D metallic phase is unusual in the sense that the usual 3D metals do not exhibit strongly temperature-dependent resistivity (unless of course there is a superconducting transition, not relevant for our consideration) at low temperatures ($T < 5$ K), the so-called Bloch-Grüneisen regime where acoustic phonon scattering (the main mechanism contributing to the temperature dependence of resistivity in bulk metals) essentially freezes out. Although phonon scattering plays a subtle (albeit secondary) role¹³ in the metallic behavior of GaAs-based (both electron and hole) 2D systems, theoretical calculations^{17,13,16} definitively show

phonon scattering to be of little significance in the observed low-temperature (≤ 1 K) 2D metallicity—in fact, in Si MOS-based 2D electron systems, where the 2D metallicity is most pronounced (and first observed), phonon scattering plays no role whatsoever in $\rho(T)$ for the experimentally relevant regime of $T < 5$ K. Phonon-scattering effects, which we have considered elsewhere^{17,13,16} in providing an explanation for the observed nonmonotonicity in $\rho(T)$ at intermediate temperatures ($T \sim 1$ –5 K) in 2D *n*- and *p*-GaAs systems, are not included in the current work since the focus of this paper is the behavior of $\rho(T)$ as $T/T_F \rightarrow 0$ where phonons surely play no role. We consider only disorder scattering due to random charged impurities (and surface roughness scattering, cf. Sec. V) in this work.

The strong temperature-dependent metallic resistivity in low-density 2D systems arise, in our view, from an interplay in the disorder scattering between finite temperature (or, even “high” temperature in the sense that $T/T_F \sim n^{-1}$ is not necessarily small as it is in 3D metals and could actually be of order unity in low-density 2D systems for $T \sim 1$ K) and density dependent 2D screening properties as reflected in the dimensionless parameter $q_{TF}/2k_F \sim n^{-1/2}$, where q_{TF} and k_F are, respectively, the 2D Thomas-Fermi screening wave vector and the Fermi wave vector.¹⁸ The fundamental difference between the semiconductor-based 2D metals of interest to us in this paper and the usual 3D metals is the great discrepancy in the magnitudes of T/T_F and $q_{TF}/2k_F$ in the two systems: In 3D metals $T/T_F \sim 10^{-4}$ for $T \sim 1$ K whereas $T/T_F \sim 0.1$ –1 in 2D semiconductor systems, and $q_{TF}/2k_F \approx 1$ in 3D metals whereas $q_{TF}/2k_F$ varies between 0.1 and 20 as carrier density is changed in the 2D systems. In addition static screening has qualitatively different wave-vector dependence in 2D and 3D systems, leading to the observed strong metallicity in various 2D systems. In 3D metals the low-temperature resistivity arises almost entirely from temperature-independent short-range disorder scattering, which leads to exponentially suppressed, $O(e^{-T/T_F})$, temperature dependence in the resistivity, and any residual small temperature dependence in $\rho(T)$ is contributed by phonon scattering [which produces the well-known Bloch-Grüneisen behavior, $\rho(T) \approx \rho_0 + AT^5$, where the temperature-independent contribution ρ_0 arises from short-range disorder scattering whereas the very weak temperature dependence characterized by the second term arises from highly suppressed phonon scattering at low temperatures]. By contrast, low-temperature transport (neglecting weak-localization effects) in 2D metallic systems of interest to us is dominated mostly by screened disordered scattering [i.e., $\rho(T) = \rho_0 + \Delta\rho(T)$ with both ρ_0 and $\Delta\rho$ being determined essentially by disorder for $T \leq 5$ K], which can be strongly temperature dependent at low densities by virtue of large possible values of the relevant parameters T/T_F (~ 1) and $q_{TF}/2k_F$ (~ 10 –20) at low densities and temperatures in 2D semiconductor structures. All localization (as well as interaction effects beyond RPA) effects are ignored² in this paper.

The paper is organized as follows. In Sec. II we discuss a scaling property (see Appendix for the theory) of the Boltzmann theory resistivity within the RPA screened charged impurity scattering model, which provides a zeroth-order quali-

tative explanation for the strength of the transport metallicity in 2D carrier systems. In Sec. III we discuss the asymptotic low-temperature ($T/T_F \rightarrow 0$) behavior of the calculated resistivity in the RPA-Boltzmann model comparing it quantitatively with the full temperature-dependent resistivity (in the same model) in order to estimate the regime of validity of the leading-order temperature expansion of resistivity. In Sec. IV we consider the various solid-state physics effects (e.g., the *quasi*-2D nature of the semiconductor layer, the long-range or the short-range nature of the *bare* scattering potential) on the 2D transport properties. In Sec. V we provide a critical comparison between our realistic (but theoretically approximate) RPA-Boltzmann 2D transport theory and a set of recent experimental results in Si inversion layer, concluding that our theory, without any adjustment of parameters and/or *ad hoc* theoretical refinement, describes well the observed experimental temperature dependence down to a carrier density of about 5×10^{11} cm⁻²—for lower densities the agreement between experiment and theory is at best qualitative with the actual temperature dependence of $\rho(T)$ being stronger than the calculated $\rho(T)$. We conclude in Sec. VI with a discussion of the implications of our results.

II. DENSITY-TEMPERATURE (q_0, t) SCALING OF METALLICITY

In the RPA-Boltzmann theory (cf. Appendix) the dimensionless r_s parameter (the so-called Wigner-Seitz radius) characterizing the electron-electron interaction strength in the 2D system does *not* play a fundamental role in determining the temperature dependence of $\rho(T)$ except so far as r_s determines the dimensionless parameters T/T_F ($\equiv t$) and $q_{TF}/2k_F$ ($\equiv q_0$) through the carrier density. We believe that the fundamental minimal parameters determining the zeroth-order 2D metallicity, i.e., the temperature dependence of $\rho(T, n)$ in the putative metallic phase are t and q_0 . In particular, for 2D systems it is easy to show that $q_0 = g_v^{3/2} r_s / \sqrt{2}$ and $t = (k_B T / Ry)(g_v / 2) r_s^2$, where g_v is the valley degeneracy of the relevant semiconductor material [$g_v = 2$ for Si(100)-MOS structures, $g_v = 1$ for *p*- and *n*-GaAs systems], $r_s = (\pi n)^{-1/2} / a_B$ is the usual dimensionless Wigner-Seitz density (or interaction) parameter with $a_B = \kappa \hbar^2 / m e^2$ as the effective semiconductor Bohr radius (κ and m are the background dielectric constant and the carrier effective mass, respectively), and $Ry = e^2 / (2 \kappa a_B)$ is the natural atomic energy unit (effective Rydberg) for the semiconductor. We find that the existing experimental data for the metallicity in various 2D semiconductor systems approximately obeys the two-parameter scaling behavior $\Delta\rho(T, n) / \rho_0 \sim F(t, q_0)$, where F is a smooth and approximately universal function of q_0 and t for all 2D metallic systems, as implied by the screening theory. In particular, a direct consequence of this theoretical prediction is that the temperature dependence of $\rho(T)$ should correlate with the parameter q_0 in different materials when expressed in terms of the dimensionless temperature t . (We note that the functional dependence of $q_0 \sim g_v^{3/2} r_s$ is not only different from the dimensionless density parameter r_s , but also from the dimensionless ratio of the Fermi energy to the Coulomb energy

in the system which goes as $g_v r_s$.) Theoretical details and the equations for our 2D RPA-Boltzmann theory are given in the Appendix of this paper where we derive this scaling law. We note that the scaling behavior $\Delta\rho/\rho_0 \sim F(t, q_0)$, with $t = T/T_F$ and $q_0 = q_{TF}/2k_F$, derived in this paper is *exact* for RPA screened charged impurity scattering in the ideal 2D limit in contrast to various other scaling behaviors (e.g., Refs. 12, 13, and 15) discussed earlier in the literature which are all approximate scaling behavior valid only in limited range of parameters.

This zeroth-order functional dependence on t and q_0 , $\Delta\rho(T, n) \equiv \Delta\rho(t, q_0)$, in fact, provides a minimal explanation for the observed strong variation in the 2D metallicity not only for various densities in the same material but for different materials at equivalent densities—for example, Si-MOSFET based 2D electron systems manifest much stronger metallicity compared with p -GaAs or n -GaAs based 2D systems even at the same r_s value because $g_v = 2$ (1) in Si (GaAs). Taking r_s to be the critical parameter determining metallicity fails to explain why the 2D p -GaAs system shows weaker metallic behavior, even though it typically has much larger r_s values ($r_s \sim 15$ – 40) than the Si system. The screening theory provides a simple explanation for this observation by virtue of q_0 being larger (by a large factor of $\sqrt{8}$) in Si than in GaAs for the same r_s value. Thus, Si MOSFET 2D metallicity at $r_s = 10$ should be approximately comparable to a GaAs 2D metallicity at $r_s = 10\sqrt{8} \approx 28$ when expressed as a function of the dimensionless temperature variable $t = T/T_F$. This predicted correspondence in the relative metallicity in terms of q_0 and t is consistent with the experimental observations in these systems. We emphasize, however, that this correspondence is expected to work only on a zeroth-order qualitative level and should not, by any means, be construed as a precise quantitative prediction. This is discussed with theoretical details in the Appendix. For example, the form factor effects associated with the quasi-2D subband quantization do not scale with the density parameter q_0 , and will necessarily affect different systems in different manners since the associated effective masses, the dielectric constants, the depletion charge densities, and the confinement potentials, which together determine the form-factor, are different in different systems. Similarly, the bare (i.e., unscreened) disorder will certainly depend on the system varying qualitatively among different systems and materials, which could lead to substantial quantitative deviations from our predicted $\rho(q_0, t)$ scaling based on the temperature-dependent screening argument. For example, in Si MOSFET's transport is dominated by interface scattering—both by long-range potential scattering due to ionized impurities located near the Si-SiO₂ interface and short-range scattering by interface roughness fluctuations inherent at the Si-SiO₂ interface. In GaAs structures (both p and n), scattering by (unintentional) background charge impurities (and less so by remote charge dopants) dominates at the highest mobilities with phonon scattering being non-negligible (although small) down to $T < 1$ K. In addition, p -GaAs structures most likely also have significant spin intersubband scattering within the spin-split valence bands. The nonuniversal quantitative ef-

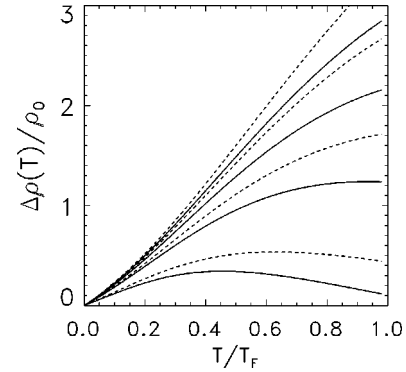


FIG. 1. Calculated $\Delta\rho = \rho(T, n) - \rho_0$, where $\rho_0 = \rho(T=0)$, for various $q_0 = q_{TF}/2k_F = 5, 10, 15, 20$ (from the bottom) as a function of $t = T/T_F$ for Si MOSFET. The solid (dashed) lines indicate resistivities from interface (bulk) charged impurities.

fects associated with subband quantization and disorder potential make the simple two-parameter screening picture of $\Delta\rho(T, n)$ dependent only on q_0 and t quantitatively inaccurate, but the simple picture applies surprisingly well on a zeroth-order qualitative level as can be verified by comparing the experimentally observed metallicity strengths in Si MOS, p -GaAs, and n -GaAs structures where the metallicity scales approximately with q_0 and t provided T is low enough so that phonon effects could be ignored in the GaAs system. The crucial point we are making in this paper is that strong metallicity manifests itself in low-density 2D systems because the control parameters $q_0 \propto n^{-1/2}$ and $t \propto n^{-1}$ are large only for low carrier densities and not because r_s is large—for example, n -Si MOS system and n -GaAs system show more than an order of magnitude different metallicities for the same r_s value because q_0 and t are much larger in Si than in n -GaAs ($\Delta\rho/\rho_0$ increases by a factor of 3 in Si MOS systems of Refs. 1 and 15 for $r_s \geq 10$ whereas it increases only by about 25% in the n -GaAs system of Ref. 16 for $r_s \geq 10$). Within a specific materials system, however, the q_0 dependence of the resistivity becomes completely equivalent to an r_s dependence (since g_v is a constant for a given system, and $q_0 \equiv g_v^{3/2} r_s / \sqrt{2}$) as one would expect—it is only in comparing different systems (e.g., Si and GaAs) that q_0 and r_s dependence are not equivalent.

In Fig. 1 we show our calculated $\rho(T, n)$, depicted in terms of the dimensionless variables q_0 and t , for a strictly 2D system using Si MOS parameters (e.g., effective mass, dielectric constant, etc.) and assuming the disorder scattering to be entirely due to finite temperature RPA-screened charged impurity scattering. Results shown in Fig. 1 demonstrate the importance of the dimensionless screening parameter $q_0 (= q_{TF}/2k_F)$ as the relevant control parameter in determining the strength of metallicity in 2D systems. In particular the maximum relative change in the resistivity $\Delta\rho/\rho_0$ ranges from about 40% for $q_0 = 5$ [which corresponds to a Si (100) inversion layer carrier density of $n = 11 \times 10^{11} \text{ cm}^{-2}$, $T_F = 80 \text{ K}$] to almost 300% for $q_0 = 20$ (corresponding to $n = 7 \times 10^{10} \text{ cm}^{-2}$, $T_F = 5 \text{ K}$) as $t \equiv T/T_F$ changes from 0 to 1 in Fig. 1. Therefore, the RPA results of Fig. 1 indicate an increase of resistivity by about 10% and

300%, respectively, for carrier densities $1.1 \times 10^{12} \text{ cm}^{-2}$ and $7 \times 10^{10} \text{ cm}^{-2}$ in Si MOSFET's for a change in T of 0–5 K, assuming that the system remains metallic. It should be noted that the maximum in $\Delta\rho/\rho_0$ shifts to higher values of t ($=T/T_F$) for higher (lower) values of $q_{TF}/2k_F$ (n), and phonon effects (ignored in our consideration) will play increasingly important quantitative role in the temperature-dependent resistivity for $T > 5$ K. These two facts together make the metallic behavior relatively even more important at lower densities, or equivalently, higher values of q_0 .

A comparison between solid and dashed lines in Fig. 1 shows the quantitative importance of the nature of impurity scattering in determining the temperature dependence of resistivity: in general, charged impurities randomly distributed in the 2D layer itself (bulk disorder shown by dashed lines in Fig. 1) lead to stronger temperature dependence than interface disorder (solid lines) associated with charged impurities distributed randomly at the semiconductor-insulator interface. This is precisely what is expected since screening effects should be the strongest when charged impurities and the carriers are distributed in the same region of space with no spatial separation. It may also be worthwhile to mention in the context of Fig. 1 that the experimental Si inversion layer systems^{1,3} manifesting the most dramatic metallicity (i.e., large changes in $\Delta\rho/\rho_0$ as a function of temperature) typically have $n \leq 10^{11} \text{ cm}^{-2}$ corresponding to $q_0 \sim 15$ –20 in Fig. 1, thereby showing a relative temperature dependent change in resistivity of about 100–300% as T/T_F varies from zero to 0.5. Thus the results in Fig. 1 are in reasonable qualitative agreement with experimental results as we have emphasized elsewhere.¹² Scattering mechanism not included in the theory (e.g., surface-roughness scattering) and higher-order interaction effects will certainly modify the quantitative details of the results, but it is gratifying to see that a zeroth-order Boltzmann transport theory including only RPA screened charged impurity scattering provides a reasonable qualitative description of the observed metallicity.

In Fig. 2 we show the calculated $\Delta\rho/\rho_0$ for three different 2D systems for a comparison of their metallicity: (100) n -Si inversion layer, p -GaAs heterostructure, and n -GaAs heterostructure. We have shown the results for the same values of carrier density, r_s parameter, and q_0 ($=q_{TF}/2k_F$) parameter in order to emphasize the importance of the dimensionless screening parameter q_0 in determining the temperature dependence. As emphasized above, for the same values of carrier density [see inset (a)], the metallicity is the strongest (weakest) in the Si (n -GaAs) system with the p -GaAs system being intermediate. For the same value of r_s parameter [see inset (b)] the metallicity depends strongly on the valley degeneracy, but weakly on the other parameters. The mass of the carrier does not change the metallicity for the same r_s parameter, which gives exactly the same resistivity behavior for p -GaAs and n -GaAs if we use the same material parameters except mass. In the main figure we show the metallicity for equivalent $q_0 = 15$ parameter values in all three systems. The thin solid line shows that the temperature dependence is scaled perfectly for the pure 2D systems, as proven in the Appendix. For quasi-2D systems, however, the scaled resistivity expressed as a function of dimensionless temperature

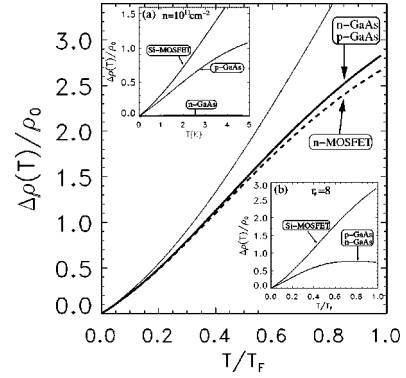


FIG. 2. The main figure shows the scaled resistivity as a function of $t = T/T_F$ for Si-MOSFET, p -GaAs, and n -GaAs with a fixed $q_0 = 15$. For pure 2D system the calculated resistivities yield perfect scaling for all systems (thin solid line). Thick lines show the scaling for quasi-2D systems. In inset (a) the comparison of the metallicity for fixed density $n = 10^{11} \text{ cm}^{-2}$ is given as a function of a temperature. In inset (b) we show the change of resistivity for fixed value of $r_s = 8$ as a function of $t = T/T_F$.

$t = T/T_F$ is approximately similar in the three systems without perfect scaling. The deviation of scaling is mostly due to form factor effects. Since the electron effective mass in n -GaAs is small ($m = 0.067m_e$), extremely low values of carrier density are required in 2D n -GaAs systems for observing appreciable screening-induced temperature dependence as has been recently reported in Ref. 16.

III. LOW-TEMPERATURE ASYMPTOTIC BEHAVIOR

Since the behavior of $\Delta\rho(T, n)$ for finite T is necessarily nonuniversal for reasons discussed above, recent attention has focused on the very low-temperature behavior of $\rho(T)$ in the $t = T/T_F \rightarrow 0$ limit. In particular, it was realized a long-time ago^{19,20} that $\Delta\rho(T, n)$ derived from the Boltzmann theory within the relaxation-time approximation for RPA screened disorder scattering has the following expansion in 2D systems:

$$\Delta\rho(T, n)/\rho_0 \approx C_1 t + C_{3/2} t^{3/2} + \dots \quad (1)$$

in the asymptotic $t \rightarrow 0$ regime. The coefficients C_1 and $C_{3/2}$ were first (but incorrectly) calculated by Gold and Dolgoplov.²⁰ We have recalculated C_1 and $C_{3/2}$, and find the original results in Ref. 20 to be incorrect. We calculate the correct coefficients (for RPA screening) to be:

$$C_1 = 2(1 + 1/q_0 f)^{-1}, \quad (2a)$$

$$C_{3/2} = 2.646(1 + 1/q_0 f)^{-2}, \quad (2b)$$

where $q_0 = q_{TF}/2k_F$ (as defined above) and $f \equiv f(2k_F)$ is the appropriate quasi-2D subband form-factor at the wave vector $2k_F$ (in general $f \leq 1$ with the strictly 2D limit being $f = 1$, see Appendix). Our calculated C_1 agrees (in the strictly 2D limit of $f = 1$) with the recent (Hartree) result given in Ref. 21 and disagree with that of Ref. 20 whose incorrectly calculated C_1 is larger by a factor of $2 \ln 2$ (i.e., about 40% higher). Our calculated $C_{3/2} \approx 2.65$ is 28% smaller in magni-

tude than the incorrect value (≈ 3.4) quoted in Ref. 20. We note that the errors in Ref. 20 led to a large overestimate of the asymptotic temperature dependence of $\rho(T)$ in the Gold-Dolgoplov formula,²⁰ which we now correct. An important recent theoretical development in the subject has been the demonstration by Zala *et al.*²¹ that the leading-order linear result given in Eq. (1), in fact, survives (albeit with C_1 replaced by an unknown Fermi-liquid parameter) inclusion of higher-order electron-electron interaction terms in the theory, of which screening is only one particular aspect. In particular, the leading-order temperature dependence in the interaction theory of Zala *et al.* contains the C_1 term of our Eqs. (1) and (2) as the so-called Hartree term in the language of Ref. 21.

A thorough understanding of this first-order linear term in the theory has taken on significance in view of the existence of the Zala *et al.*²¹ work, and even more importantly, because of the several recent attempts^{11,22,23} to compare experimental results to the interaction theory. The interaction theory considerably extends the screening theory (through the inclusion of higher-order interaction corrections), but is unfortunately constrained at this stage to only the leading order result in t , and therefore applies only at very high (low) densities (temperature) so that the constraints $t \ll 1$ and $\Delta\rho/\rho_0 \ll 1$ are satisfied. The two theories are thus complementary—the screening theory being an approximate theory (because it includes only the screening part of the electron-electron interaction) for *all* t (in fact, its accuracy improves with increasing t since the RPA becomes exact in the classical high-temperature limit) whereas the interaction theory is presumably an exact leading-order in t (within the perturbative Landau Fermi liquid theory scheme) theory as $t \rightarrow 0$. This obvious complementarity of these two approaches has not been emphasized in the recent literature where some recent publications have even presented the misleading and incorrect viewpoint of these two approaches as mutually exclusive competing theories. It is important to emphasize that the interaction theory,²¹ by construction, applies only when the temperature correction to the $T=0$ conductivity is small, i.e., the theory of Ref. 21 is a leading order theory for small temperature corrections to the $T=0$ conductivity as $T/T_F \rightarrow 0$. By definition, therefore, this interaction theory cannot explain the strong metallicity or the large temperature-dependent changes in the resistivity reported in the literature. The real significance of Ref. 21 is strictly theoretical—it shows that the metallic behavior given by Eq. (1) within the RPA-Boltzmann theory survives higher-order electron-electron interaction corrections in the $T/T_F \rightarrow 0$ limit [provided that the “ballistic” transport condition $k_B T \gg \hbar/\tau$, where τ is the $T=0$ transport relaxation time ($\tau = m/ne^2\rho_0$), is satisfied, i.e., the temperature is in the intermediate range $T_F \gg T \gg \hbar/\tau k_B$]. We note that the necessary condition minimally required for a comparison between experiment and the interaction theory is that (1) the experimental conductivity must show a linear temperature correction in the intermediate temperature regime $T_F \gg T \gg \hbar/\tau k_B$, and (2) the temperature correction to the $T=0$ conductivity must be small. Most experiments on 2D transport do not satisfy these necessary conditions for comparison with the interaction theory, most particularly because

the measured conductivity essentially never manifests a linear temperature dependence except at very high densities where the RPA-Boltzmann semiclassical transport theory is quantitatively accurate.

In view of the complementary nature of these two theories it becomes important to ask about the regime of validity of the linear approximation inherent in the interaction theory. This issue becomes particularly crucial since most of the existing $\rho(T)$ data in the putative 2D metallic phase does not follow a linear temperature dependence over any appreciable temperature regime in the lowest-temperature range (i.e., $T/T_F \ll 1$). The situation becomes more complicated with the realization that the “strong” condition (the “weak” condition being $T \ll T_F$) for the validity of the interaction (as well as the screening) theory is that $T_D \ll T \ll T_F$, where $T_D \approx \hbar/(\tau k_B)$ is roughly the so-called Dingle temperature with τ being the $T=0$ limit of the transport relaxation time [i.e., $\tau = m/(ne^2\rho_0)$]. In the screening theory T_D cuts off the temperature dependence of screening for $T \leq T_D$ (making the disorder to be effectively temperature independent for $T \ll T_D$) leading to a suppression in the temperature dependence of $\rho(T)$ whereas the interaction theory is by construction a theory of ballistic transport developed in the $\hbar/(\tau k_B T) \ll 1$ limit (and then the $T/T_F \ll 1$ limit is taken to obtain explicit asymptotic results). The T_D cutoff in the temperature dependence of $\rho(T)$ for $T \leq T_D$ is extremely well-motivated physically within the screening theory, and has been discussed in details in the literature^{12,13,19} as the reason for the need of low disorder (or equivalently, high mobility with concomitant low values of T_D) samples to observe 2D metallicity (low density is also required in the screening theory for strong metallicity so as to produce large values of T/T_F at low temperatures and to make $q_{TF}/2k_F$ large enough to have strong screening effect). We will mostly ignore the Dingle temperature effects in the theory by assuming $T_D \approx 0$, but in comparing experimental data to the interaction theory the ballistic limit is an important constraint to remember. In particular, in many experimental situations the constraint $\hbar/(\tau k_B) \ll T \ll T_F$ necessary for the application of the ballistic limit interaction theory may not even exist.²³

To address the important question of the regime of validity of the asymptotic linear approximation we have carried out a careful comparison between the linear- T approximation [Eqs. (1) and (2)] and the full numerical calculation of $\rho(T)$ within the RPA-Boltzmann theory. (These results are presented in Figs. 3 and 4.) The important conclusion drawn from this comparison is that the regime of validity of the asymptotic linear formula, $\Delta\rho/\rho_0 \sim O(T/T_F)$, is extremely restricted, and at least for the RPA screened disorder scattering, the linear approximation holds only in the very low-temperature limit of $T/T_F < 0.05$, which, in general, is not in the ballistic regime except at very high densities where the metallicity is very weak. We therefore conclude that the low-temperature asymptotic linear regime, while being of substantial theoretical interest, is not of much experimental relevance since $\Delta\rho \sim T$ only for temperatures (densities) much too low (high) to be of experimental interest. Our conclusion is based on a comparison of the asymptotic analytic linear- T formula with the full T -dependent calculation only for the

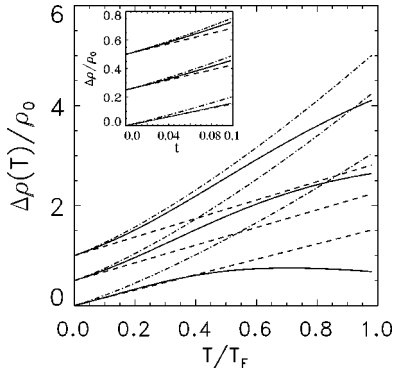


FIG. 3. $\rho(T)$ for a Si-MOSFET with density $n=56.0, 12.0, 7.0 \times 10^{10} \text{ cm}^{-2}$ (from the bottom). Solid lines indicate the full RPA screening theory, dashed lines the asymptotic approximations with only the linear term, and dot-dashed lines with both the $O(T)$ and $O(T^{3/2})$ terms. For clarity we use offset by 0.5 for lower densities. The inset shows $\rho(T)$ on an expanded temperature scale.

RPA screening theory (because this is the only theory where both the asymptotic result and the full result can be calculated), but we believe our conclusion to be quite generally valid, and even for the interaction theory we expect the low- T regime of validity of the linear T formula to be too restricted to be of much experimental relevance. This is consistent with the existing experimental results where the conductivity is never precisely linear (at low temperatures) essentially at any carrier densities, except perhaps at very high carrier densities where the RPA-Boltzmann theory should be quantitatively valid.

In Fig. 3 we show our calculated $\rho(T)$ for three densities in the (100)Si MOS 2D electron system in both the full RPA screening theory and in the asymptotic approximations keeping only the leading-order linear term and both the $O(T)$ and $O(T^{3/2})$ terms in Eq. (1). We have assumed scattering from a random distribution of charged impurities located at the interface, and subband form-factor effects have been included in both calculations equivalently. The inset shows $\rho(T)$ on an expanded temperature scale.

In Fig. 4 we show similar comparisons between the calculated full $\rho(T)$ and the asymptotic analytic approximations for 2D GaAs holes and electrons in their experimentally relevant density regimes of interest. For these two systems we show results for two different impurity scattering mechanisms for the sake of completeness (also for the sake of consistency with the experimental GaAs systems where interface charged impurity scattering is typically less important than in Si MOSFET's). In particular, we give results for scattering by a uniform random distribution of (unintentional) background ionized impurities (which are invariably present and are usually the dominant scattering centers in the GaAs samples of the highest mobilities) and by remote charged dopants (assumed to be randomly distributed in a 2D plane separated a modulation distance of d from the 2D electron layer), the so-called modulation doped situation. It is obvious from Fig. 4 that 2D n -GaAs system not only has the weakest temperature dependence but also exhibits essentially no clear linear temperature regime. This is consistent with the very weak screening properties (and large values of E_F) of 2D

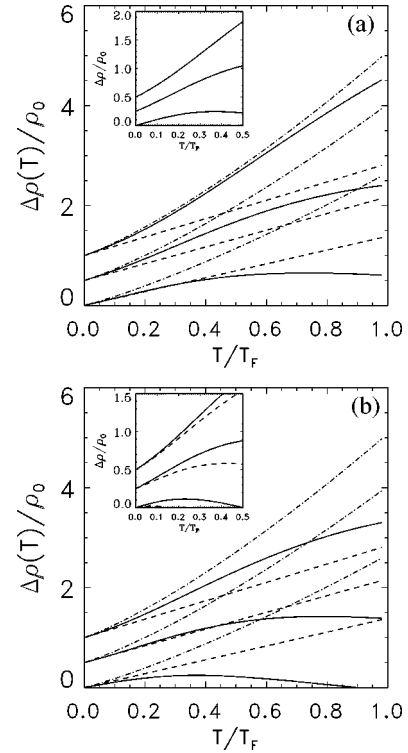


FIG. 4. Calculated $\rho(T)$ as a function of $t=T/T_F$ (a) for p -GaAs with density $n=21.8, 5.45, 1.36 \times 10^{10} \text{ cm}^{-2}$ (from the bottom) and (b) for n -GaAs with density $n=6.1, 1.5, 0.38 \times 10^9 \text{ cm}^{-2}$ (from the bottom) by considering only scattering from a uniform random distribution of ionized impurities in the quantum well. Solid lines indicate the full RPA screening results, dashed lines the asymptotic approximations with only the linear term, and dot-dashed lines with both the $O(T)$ and $O(T^{3/2})$ terms. Offset by 0.5 for lower densities is used. The inset in (a) shows $\rho(T)$ for charged impurities at interface. The inset in (b) shows $\rho(T)$ for scattering by remote charged dopants at $d=100 \text{ \AA}$ (solid lines) and $d=300 \text{ \AA}$ (dashed lines) on an expanded temperature scale.

n -GaAs because of its very low band effective mass. The real importance of the actual random impurity distribution in the system (usually not known and has to be inferred from a comparison of the transport data with theoretical calculations assuming specific impurity distributions) in affecting (both qualitatively and quantitatively) the $\rho(T)$ behavior is apparent in the results of Fig. 4: The strongest temperature dependence arises in the situation where the charged impurities are randomly distributed in the 2D layer of the carriers and the weakest T dependence arises in the modulation doped situation (particularly for densities low enough so that $2k_F d \geq 1$) with the interface disorder case being intermediate. This dependence on the details of disorder is easily understood within the screening theory by considering the role of $2k_F$ scattering in transport: Modulation doping with $2k_F d \geq 1$ essentially completely suppresses large momentum $2k_F$ scattering even at low temperatures because of the $e^{-2k_F d}$ term in the form factor drastically reducing the temperature dependence due to screened impurity scattering whereas charged impurities distributed randomly in the 2D layer maximizes $2k_F$ scattering for a given system. The interaction

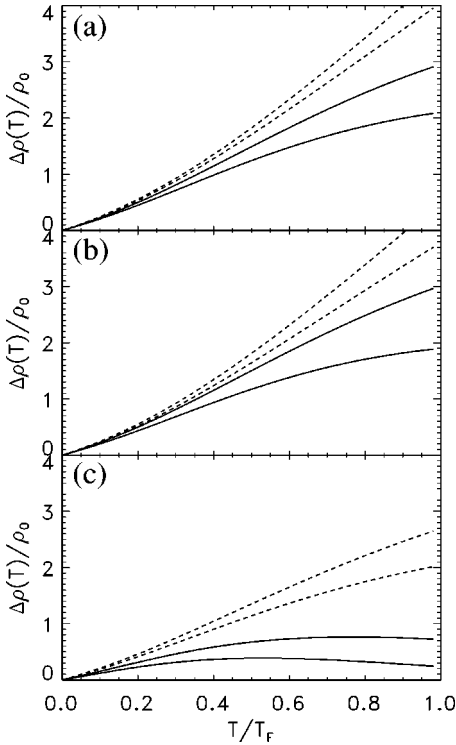


FIG. 5. The calculated pure-2D (dashed lines) and quasi-2D (solid lines) temperature-dependent resistivity for screened bulk charge impurity scattering (a) for Si-MOSFET with $n=10, 20 \times 10^{10} \text{ cm}^{-2}$, (b) for p -GaAs with $p=2.0, 5.0 \times 10^{10} \text{ cm}^{-2}$, and (c) for n -GaAs with $n=0.5, 1.0 \times 10^{10} \text{ cm}^{-2}$. The lower lines represent higher densities.

theory of Zala *et al.*²¹ had to make the drastic approximation of a zero-range white-noise impurity disorder potential, thus drastically (and artificially) enhancing the $2k_F$ scattering. In real systems, other things being equal (i.e., the mobility, the density, and the 2D system), there would be a strong dependence of the detailed behavior of $\rho(T)$ on the actual random impurity distribution in the system through the form-factor effect. (Note that the low- T asymptotic linear formula does not depend on the impurity distribution or on the range of disorder scattering, but its temperature regime of validity may very well depend on the nature of scattering in the 2D system.)

IV. SOLID-STATE PHYSICS EFFECTS: QUASI-2D LAYER WIDTH AND BARE IMPURITY POTENTIAL RANGE

We now discuss the quantitative significance of various solid-state physics effects on the 2D metallicity. The specific effects we discuss are the quasi-2D nature of the semiconductor layers under consideration and the nature of bare impurity disorder (i.e., long range versus short range) in determining the temperature dependence of 2D resistivity. (Both of these effects are ignored in Ref. 21. The inclusion of the quasi-2D form-factor effect in the interaction theory is straightforward, but the inclusion of long-ranged bare disorder, e.g., charged impurity scattering, in the interaction theory is nontrivially difficult.) In Fig. 5 we compare the

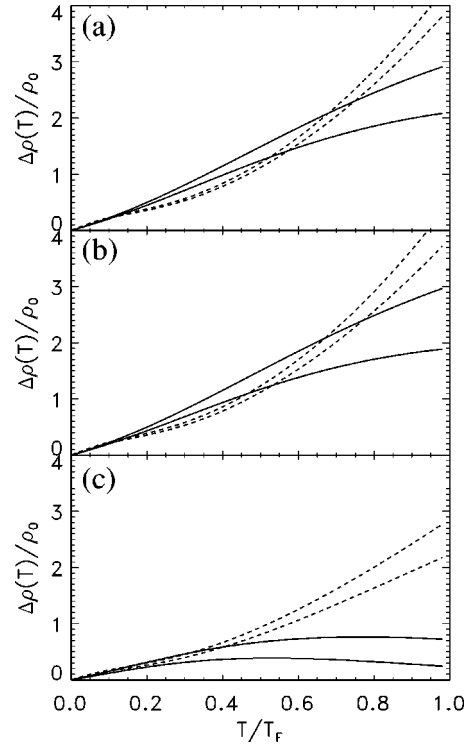


FIG. 6. The calculated temperature-dependent resistivities for realistic long-range charged impurity scattering (solid lines) and for hypothetical short-range δ -function impurity scattering (dashed lines) (a) for Si-MOSFET with $n=10, 20 \times 10^{10} \text{ cm}^{-2}$, (b) for p -GaAs with $p=2.0, 5.0 \times 10^{10} \text{ cm}^{-2}$, and (c) for n -GaAs with $n=0.5, 1.0 \times 10^{10} \text{ cm}^{-2}$. The lower lines represent higher densities.

calculated 2D and quasi-2D temperature-dependent resistivity for screened bulk charge impurity scattering, finding that the metallicity is substantially overestimated in the strictly two-dimensional approximation. Thus, it is essential to include the quasi-2D nature of the semiconductor system in order to obtain quantitatively accurate temperature dependence although the 2D approximation is qualitatively correct.

In Fig. 6 we show a comparison between the results calculated for realistic long-range charged impurity scattering and hypothetical short-range δ -function (in real space) impurity scattering (both equivalently screened by the finite temperature RPA dielectric function of the 2D carriers). We point out that the dominant disorder in 2D semiconductor systems arises from long-range (Coulomb) charged impurity scattering. In Fig. 6, the calculated temperature dependence is obviously substantially stronger for short-range bare disorder. It is important to emphasize in this context that the leading-order asymptotic dependence of $\Delta\rho/\rho_0$ on T/T_F is *independent* of the range of the bare disorder since it depends [see Eqs. (1) and (2)] on the electron-impurity interaction only through $V_{e-i}(2k_F)$, i.e., through the constant (momentum space) impurity potential defined at the wave vector $q = 2k_F$, making long- and short-range bare disorder completely equivalent for the low-temperature asymptotic temperature dependence. On the other hand, the full temperature dependence depicted in our Fig. 6 manifestly demonstrates that, except at the lowest values of $t = T/T_F \leq 0.1$, the actual

temperature-dependent resistivity depends quite significantly on the range of bare disorder with short-range bare disorder providing substantially stronger temperature dependence than the long-range Coulomb disorder due to random charged impurity scattering. Since we have already argued in Sec. III that the asymptotic linear temperature dependence does not really apply, except at extremely low temperatures (or high carrier densities), the range of impurity disorder potential takes on special significance in the theoretical analyses.

V. COMPARISON WITH EXPERIMENT

Although the primary goal of this article is to establish and clarify certain theoretical principles (e.g., the validity of the asymptotic low-temperature expansion, the strength of metallicity as reflected in the q_0 , t_0 scaling behavior, the importance of various realistic solid-state physics effects such as the long-range versus the short-range nature of the bare impurity disorder potential or the quasi-2D nature of the semiconductor systems of experimental interest) within the RPA-Boltzmann theory of 2D carrier transport in semiconductor systems, it is important to ask about the empirical validity of the zeroth-order RPA-Boltzmann theory in the context of the large amount of the available temperature-dependent 2D transport experimental data. We have in fact carried out a number of comparisons between our theory and the experimentally measured temperature-dependent resistivity in several different 2D systems of current interest.^{12–16,23,25–27} It is important in this context to remember that such comparisons between experiment and theory is necessarily qualitative in nature since the experimental data, even in the same material system, show strong sample to sample variations, and the measured $\rho(T, n)$ in different Si MOS systems (or for that matter, in different n -GaAs or p -GaAs systems) often have significantly different quantitative (and sometimes even qualitative) dependence on temperature and carrier density. This is understandable since different samples in general may have significantly different bare disorder potential and system parameters, and therefore a universal quantitative behavior of $\rho(T, n)$ cannot be expected (since there is no universal quantitative behavior for the experimental data themselves).

The important question therefore is the extent to which a particular theory explains the qualitative behavior of the observed $\rho(T, n)$ in 2D systems. The RPA-Boltzmann theory discussed in this paper is unique in this respect since it is the *only* theory which is capable of producing the full temperature and density dependent 2D resistivity which can, in principle, be compared with the experimental data. The theory is still not uniquely defined since all the system parameters (e.g., effective mass, depletion charge density, the precise metallic carrier density, etc.) are never really accurately known, and more importantly, the detailed quantitative parametrization of the bare disorder potential is never available for any sample. In general, there could be many independent sources for the bare disorder (e.g., bulk and interface charged impurities, surface roughness, remote impurities, intervalley scattering, phonons, alloy scattering), and with a sufficient

number of adjustable free parameters characterizing different kinds of disorder assumed to exist in a system one may very well be able to obtain essentially complete (but, meaningless) agreement with experimental data for any particular sample.

With all these caveats in mind we carry out a comparison between our theory and a recent set of experimental data²² for $\rho(T, n)$ in a Si MOS system. The specific sample we choose for this comparison is the Si-22 sample [see Fig. 1(a) of Ref. 22] with a quoted “peak mobility” of $33\,000\text{ cm}^2/\text{Vs}$. In Ref. 22 a series of $\rho(T)$ curves, for $T \approx 0.5\text{ K}–5.0\text{ K}$, are presented for this sample in the 2D carrier density range of $n = (5.7–35.7) \times 10^{11}\text{ cm}^{-2}$ with the typical resistivity values spanning between $0.002\text{ } h/e^2$ to $0.02\text{ } h/e^2$. The temperature induced fractional change in $\rho(T)$ in this $0.5–5.0\text{ K}$ temperature window spans between a few percent at higher densities to about 35% at the lowest densities. Visually the $\rho(T)$ curves of Fig. 1(a) in Ref. 22 corresponding to the Si-22 sample all seem to obey the asymptotic linear temperature dependence although, in general, there is significant deviation from linearity *both* at the lowest ($\leq 0.5\text{ K}$) and at the highest ($\leq 5\text{ K}$) temperatures.

In Figs. 7 and 8 we show our calculated $\rho(T, n)$ for the Si-22 sample²² within the RPA-Boltzmann transport theory assuming screened disorder scattering. In Fig. 7(a) we show the calculated RPA-Boltzmann resistivity, assuming only interface (or oxide) charged impurity scattering, for all the densities corresponding to Fig. 1(a) in Ref. 22. The results shown here look qualitatively similar to the experimental data [cf. Fig. 1(a) in Ref. 22] except that the temperature dependence is somewhat weaker in the theory. In Fig. 7(b) we show the theoretical results, $\rho(T)$ with $T = 0.25–6\text{ K}$, for six representative carrier densities $n = 5.7, 6.9, 8.7, 11.7, 16.5, 35.7 \times 10^{11}\text{ cm}^{-2}$ (top to bottom in Fig. 7) using impurity scattering as the only resistive mechanism in the system, comparing the quasi-2D realistic situation and a long-range bare impurity potential with the idealized 2D situation and a short-range bare impurity potential. The two sets of calculated results in Fig. 7 corresponding to the realistic quasi-2D system (with finite 2D layer thickness, semiconductor-insulator dielectric mismatch, etc.) with long-range bare Coulomb impurities randomly distributed at the interface (dashed lines) and the ideal zero-thickness 2D layer approximation with zero-range δ -function potential *bare* impurity scatterers (the model, for example, of Ref. 21) providing the resistive scattering mechanism (solid lines). We note several important features of the results presented in Fig. 7: (1) The theoretical results for $\rho(T)$ appear to be approximately linear in T for all the carrier densities, being qualitatively very similar to the experimental data shown in Fig. 1(a) of Ref. 22; (2) in spite of this qualitative linearity of $\rho(T)$, the actual curves are nonlinear except at the highest densities; (3) an approximate measure (actually a lower bound) of this nonlinearity is the difference between the solid and dashed lines in Fig. 7 since the slopes of the two lines are the *same* in the $T \rightarrow 0$ limit where both are strictly linear in T/T_F as discussed above in Sec. III; (4) the calculated results, while being qualitatively similar to the data,²² disagree quantitatively with experiment with the quantitative disagreement

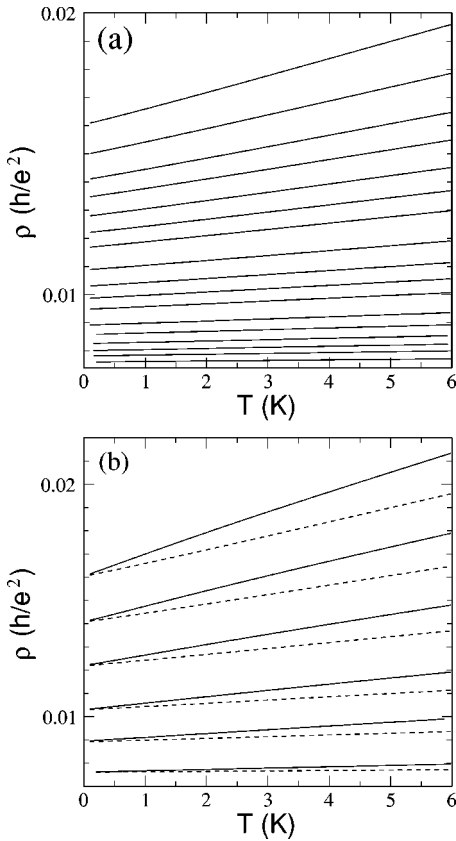


FIG. 7. (a) Calculated $\rho(T, n)$ within the RPA-Boltzmann transport theory assuming only interface charged impurity scattering, for all the densities corresponding to Fig. 1(a) (Si-22 sample) in Ref. 22. (b) Calculated $\rho(T, n)$ with long-range Coulomb impurities randomly distributed at the interface (dashed lines) and the ideal zero-thickness 2D layer approximation with zero-range δ -function potential bare impurity scatterers (solid lines) for six representative carrier densities $n = 5.7, 6.9, 8.7, 11.7, 16.5, 35.7 \times 10^{11} \text{ cm}^{-2}$ (top to bottom).

increasing with decreasing carrier density; (5) the *unrealistic* strictly 2D approximation with zero-range δ -function bare disorder potential (solid lines in Fig. 7) actually agrees much *better* with the experimental data than the realistic quasi-2D calculation with charged Coulomb impurity scattering as the bare disorder (dashed lines) since the experimental data of Ref. 22 *shows* stronger temperature dependence quantitatively than the theoretical results of Fig. 7 (again this is consistent with the discussion of Sec. IV above where δ -function bare impurity disorder and/or strict 2D approximation turns out to give much stronger temperature dependence than the realistic quasi-2D system with charged Coulomb scattering)—we emphasize, however, that both the solid and the dashed lines have the same slope in the $T/T_F \rightarrow 0$ limit reinforcing the lack of linearity in the $\rho(T)$ behavior.

To go beyond the qualitative agreement with experiment depicted in Fig. 7, we consider in Fig. 8 a *more realistic* situation taking into account, in addition to the charged Coulombic impurity disorder, the surface roughness scattering by the Si-SiO₂ interface which has been known for a very long

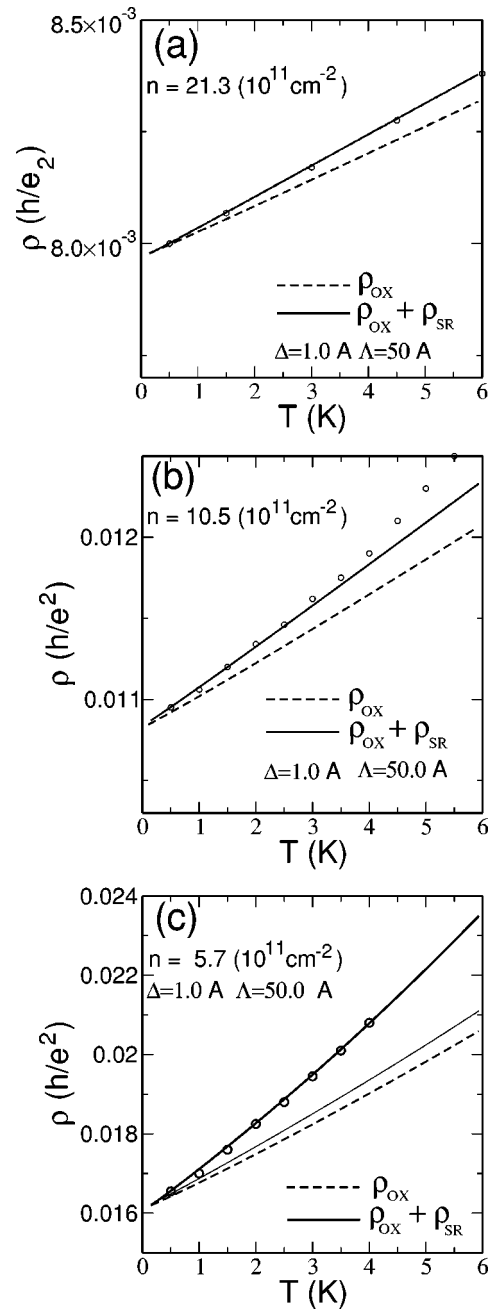


FIG. 8. Calculated $\rho(T)$ for three carrier densities (a) $n = 21.3 \times 10^{11} \text{ cm}^{-2}$, (b) $n = 10.5 \times 10^{11} \text{ cm}^{-2}$, (c) $n = 5.7 \times 10^{11} \text{ cm}^{-2}$, including realistic surface roughness and interface (oxide) charged impurity scattering. In (c) the thin (thick) solid line represents the result using the band effective mass (the measured effective mass from Ref. 24). Here Δ is the average displacement of the interface and Λ is of the order of the range of its spatial variation in the direction parallel to the surface.

time¹⁸ to be the dominant scattering mechanism affecting carrier transport in Si MOSFET's at relatively "higher" carrier densities whence the 2D electron gas resides rather close to the Si-SiO₂ interface making the roughness scattering to be significant. We include the surface roughness scattering in our theory in the standard manner,¹⁸ screening it within the RPA theory similar to the charged impurity scattering

theory.¹⁹ In Figs. 8(a)–8(c) we show our calculated $\rho(T)$ for three representative carrier densities (all for the Si-22 sample of Ref. 22) $n = 5.7, 10.5, 21.3 \times 10^{11} \text{ cm}^{-2}$ including realistic surface roughness and interface (oxide) charged impurity scattering. At higher densities the quantitative agreement between the realistic calculations (solid lines) including both charged impurity and surface roughness scattering and the experimental data is very good whereas at the lower density ($5.7 \times 10^{11} \text{ cm}^{-2}$) the agreement is systematically poorer at higher temperatures where the theory consistently underestimates the experimental temperature dependence. However, if we use the actual density dependent effective mass measured in the experiment rather than the band mass, we obtain much better agreement between our result and the experimental data at low densities. In Fig. 8(c) we show our calculated resistivity (thick solid line) using the measured effective mass taken from Ref. 24. We note, however, that the effective mass renormalization (and its effect on transport) is a rather subtle issue, and, in spite of the excellent quantitative agreement obtained in Fig. 8(c) using the experimentally measured density dependent effective mass, it is unclear whether the band mass or the renormalized mass should be used in our RPA-Boltzmann transport theory.

The quantitative agreement shown in Fig. 8 can be further improved by including *bulk* charged impurity scattering due to random ionized impurity centers in the semiconductor material itself, whose relative importance increases at lower densities as the 2D electrons reside on the average more deeply inside Si (and away from the interface). If we include in addition scattering by *neutral* impurities (with short-range bare impurity potential in contrast to the long-range bare impurity potential arising from the charged impurities), we can essentially obtain quantitative agreement between theory and experiment by suitably adjusting the relative impurity densities among oxide charged impurities, bulk ionized impurities, and neutral short-range impurities (in addition, of course, to short-range surface roughness scattering). But such a parametrized quantitative agreement between theory and experiment is essentially a device simulation exercise and is completely meaningless from the perspective of the fundamental physics of 2D carrier systems, since it does not tell us anything more than what the results of Figs. 7 and 8 already tell us. The important point to realize here is that even the qualitatively valid results of Fig. 7 already show the same level of *quantitative* agreement between the RPA-Boltzmann theory and the Si-22 data of Ref. 22 as the existing agreement among the experimental data from different Si MOSFET samples at same densities and temperatures—this can be easily seen just by comparing to the data in Fig. 1(a) of Ref. 22 corresponding to the Si-22 sample with those in Fig. 1(b), 1(c) of Ref. 22 corresponding to the Si-15 sample (in fact, sample to sample variations in the observed $\rho(T, n)$ in various Si MOSFET's are typically much larger than the quantitative agreement we find without adjusting any parameters in Fig. 8). Our results shown in Figs. 7 and 8 also reinforce the real danger of insisting just on “explaining” theoretically the low-temperature slope of the resistivity (which automatically assumes a linear temperature dependence in both resistivity and conductivity) as has been fash-

ionable in the recent experimental work^{11,22} motivated by the asymptotic low-temperature analysis of the interaction theory.²¹ As Figs. 7 and 8 explicitly demonstrate, an agreement between theory and experiment on $d\rho/dT$ in the $T \rightarrow 0$ limit is absolutely no guarantee for a quantitative agreement between theory and experiment in a reasonable temperature range. Finally, we point out that the unrealistic ideal 2D approximation and bare zero-range disorder potential misleadingly provides “better” quantitative agreement between theory and experiment, which of course does not mean anything about the physics of 2D carrier systems. We also note in this context that the quantitative agreement between the RPA-Boltzmann theory and the low-density experimental data can be substantially improved¹² by assuming an effective lower density for the *free* carriers (participating in metallic transport) than the nominal 2D carrier density, which is equivalent to invoking a lower effective Fermi temperature for the system (this could also arise from an enhanced effective mass at lower densities as has been experimentally observed), thus effectively enhancing the theoretical temperature dependence.

It is instructive to separate on the possible reasons for the systematic deviation of the experimental $\rho(T)$ from the RPA-Boltzmann theory at lower densities ($\leq 5 \times 10^{11} \text{ cm}^{-2}$) and moderate temperatures ($\geq 2 \text{ K}$). There are two general possibilities: limitation or shortcomings of the RPA-Boltzmann theoretical scheme and the participation of scattering mechanisms left out of our model. The RPA-Boltzmann transport theory is obviously quite approximate since it is fundamentally semiclassical in nature leaving out all interaction, localization, and quantum interference effects. It is, however, difficult to understand why these effects (i.e., localization, interaction, interference), which are left out of the RPA-Boltzmann transport theory, would become quantitatively more important at higher temperatures. In fact, quantum effects should be progressively weaker as T/T_F increases, and therefore the systematic underestimation of the experimental $\rho(T)$ in our RPA-Boltzmann theory is very unlikely to arise from the theoretical approximations of our model. We believe that the systematic apparent disagreement between experiment and theory at higher temperatures and lower densities in Fig. 8, if real, must arise from a missing scattering mechanism (neglected in our model) which takes on significance at higher temperatures. Such additional (high-temperature) scattering may be due to intervalley scattering in Si and/or surface/oxide phonon modes not included in our theory.

In discussing the theoretical approximations of our model it is important to emphasize, particularly in the context of the results shown in Figs. 7 and 8 for comparison with the data of Ref. 22, that the leading-order single-site scattering approximation used in our theory is quite accurate since the typical values of “ $k_F l$ ” (where k_F and l are, respectively, the Fermi wave vector and the carrier mean free path) are rather large for the results depicted in Figs. 7 and 8. It is easy to show that for a 2D system $k_F l = \tilde{\sigma}/g_\nu$, where $\tilde{\sigma} \equiv \sigma/(e^2/h)$ is the dimensionless conductance of the 2D system. For the results of Ref. 22, as shown in Figs. 7 and 8 of our paper, $k_F l$ is typically 100 or higher, making the single-site approxima-

tion well valid. Thus, we do not believe that higher-order impurity scattering effects (or localization effects) are important in the regime of density and temperature covered in our Figs. 7 and 8. Obviously, at lower densities, near the critical density for the metal-insulator transition (where $k_F l \leq 1$), higher-order impurity scattering effects become very important, and our simple RPA-Boltzmann theory breaks down.

VI. DISCUSSION AND CONCLUSION

We have carried out a critical comparison between the full $\rho(T)$ calculated within the RPA-Boltzmann theory and its asymptotic ($T/T_F \rightarrow 0$) linear- T approximation, finding that the linear approximation strictly applies only at very low temperatures, typically $T/T_F < 0.05$, at least within the RPA screening theory. In addition, we have provided a qualitative explanation, based on our approximate finding $\Delta\rho(T, n) \approx \Delta\rho(t, q_0)$ where $t \equiv T/T_F$ and $q_0 \equiv q_{TF}/2k_F$, for the relative strength of metallicity in various 2D systems (showing in the process that the dimensionless screening parameter q_0 , and *not* the dimensionless interaction parameter r_s , provides a better zeroth-order qualitative description for the metallicity trend in various materials). We have also carried out a detailed analysis of $\rho(T, n)$ in the strictly 2D limit (i.e., with the subband form factor $f \equiv 1$) and using short-range bare disorder. The strictly 2D results are in general quantitatively incorrect showing a more prominent linear low- T regime and manifesting much stronger metallicity than the realistic quasi-2D results. Similarly, the short-range bare disorder manifests stronger temperature dependence than the realistic charged impurity scattering case although they both have the same leading-order temperature dependence. We have also carried out our theoretical transport calculations (not presented in this paper) including local-field corrections to 2D screening by going beyond RPA (which is exact only in the high density or in the high-temperature limit). Our results with local-field corrections are qualitatively very similar to the RPA screening results presented in this paper except that the temperature dependence of $\rho(T)$ is in general somewhat weaker. We restrict ourselves to presenting only RPA screening results because there is no unanimity in the literature about the best possible local-field corrections and also because the temperature dependence of local-field effects are in general unknown. We point out that recent experiments attempting to verify the interaction theory^{11,22,23} have produced conflicting results mainly because a clear linear- T regime in conductivity satisfying $T_D \ll T \ll T_F$ seems not to exist in low density metallic 2D systems (as we explicitly show for the screening theory results in this paper) in any experimentally accessible range of the low- T data. One should therefore be extremely careful in applying any leading-order asymptotic temperature expansion to the 2D resistivity in analyzing experimental data.

This caution in comparing 2D transport data with the interaction theory²¹ is particularly warranted in view of the minimal necessary (but by no means sufficient) conditions that must be satisfied for such a comparison to be meaningful: (1) The weak temperature constraint $T_D \ll T \ll T_F$ must be obeyed so as to be in the low-temperature ballistic limit and

phonon scattering must be negligible; (2) a clear linear temperature dependence in the low-temperature conductivity (not resistivity) $\sigma(T) = \sigma_0[1 + C_1(T/T_F)]$, where the slope C_1 depends on density, must be observed over a *reasonable* (a decade or more) range of temperature satisfying the ballistic constraint $T_D \ll T \ll T_F$; (3) the actual temperature dependent conductivity correction, $\Delta\sigma/\sigma_0 = |\sigma(T) - \sigma_0|/\sigma_0$, must be very small ($\Delta\sigma/\sigma_0 \ll 1$) for the leading-order interaction theory to be applicable. This set of necessary conditions is sufficiently restrictive so that no 2D transport experiment actually satisfies all three conditions except at very high carrier densities where the RPA-Boltzmann theory gives quantitatively accurate results.²⁷

Before concluding we discuss the experimental relevance of our (q_0, t) scaling prediction and the theoretical relevance (or validity) of our RPA screening approximation. A cursory examination of the available 2D transport data shows that our predicted scaling of $\Delta\rho/\rho_0$ with the parameters $q_0 = q_{TF}/2k_F$ and $t = T/T_F$ works on a qualitative level as a zeroth-order description for GaAs electrons and holes, and also for electrons in Si MOS but only at low values of T/T_F (≤ 0.2). At higher temperatures phonon scattering becomes significant^{13,16,23} in 2D GaAs systems whereas in Si MOS structures, where phonon effects should be negligible, the temperature dependence of resistivity at lower metallic densities becomes stronger than our prediction for reasons unclear to us. We note that this systematic underestimation of experimental temperature dependence of $\rho(T, n)$ at lower (higher) values of n (T) in the RPA scattering theory is unlikely to be arising from the interaction effects considered in Ref. 21 since the disagreement arises in the nonasymptotic regime of $T/T_F \geq 0.2$ where the experimental $\rho(T, n)$ is manifestly nonlinear in T/T_F making the theory of Ref. 21 inapplicable. We can speculate several possible reasons for this unusually strong temperature dependence of Si MOS-FET's: (1) Somehow the effective Fermi temperature (and the Fermi wave vector) in the system could be smaller than the nominal Fermi temperature (or the Fermi wave vector) obtained on the basis of (100) Si inversion layer band mass and measured carrier density (leading to enhanced values of q_0 and/or t)—for example, the effective mass could be larger due to renormalization or the effective free carrier density smaller (e.g., due to trapping by interface defects); (2) there could be additional scattering mechanisms (e.g., intersubband scattering between different valleys in Si, which would be enhanced at higher temperatures) not included in our theory; (3) RPA could be failing systematically at higher values of T/T_F (this is an unlikely scenario since RPA should become a better approximation at higher T/T_F values, and going beyond RPA including local-field corrections does not help in this respect).

We note that we have ignored in this work any damping correction to the RPA screening function arising from the impurity scattering effect. In particular, for $T \ll T_D$ the temperature-induced thermal suppression of $2k_F$ screening, which is crucial in producing the strong temperature dependence of resistivity¹⁹ at low temperature, becomes completely ineffective since collisional broadening or damping effects induced by impurity scattering already suppresses

screening at $q=2k_F$. Therefore, for $T \ll T_D$ we expect the 2D resistivity $\rho(T)$ to become essentially independent (or a very weak sublinear function) of temperature. This is, in fact, precisely the experimental observation—the strong (and often approximately linear) temperature dependence of the low-temperature resistivity almost always shows a saturation at very low temperatures for $T \ll T_D$. This damping or broadening induced screening suppression for $T \ll T_D$ has a more subtle effect also. At low carrier densities T_F is low and T_D is typically high since scattering effect is strong at low density; therefore at very low densities, a metallic 2D system may not manifest strong metallicity because the damping induced low-temperature saturation of $\rho(T)$ will be more important as T_D approaches T_F at low densities. This effect is also consistent with experimental observations. We have discussed elsewhere¹² the damping correction to screening in some details in the context of the 2D metal-insulator-transition (MIT) phenomenon. In this article we have restricted ourselves mostly to discussing the ballistic $T \gg T_D$ regime of 2D metallicity, and as such, we have decided to ignore the damping correction. The other reason for ignoring the damping correction is that the precise Dingle temperature value T_D to be used in the theory is unknown, and therefore it introduces an unknown free parameter which we wish to avoid. Also, our purpose of comparison with the interaction theory of Zala *et al.*²¹ is not well served by having the damping correction since the interaction theory has been explicitly developed for the ballistic regime. We do mention, however, that introducing a Dingle temperature induced damping correction to the RPA screening function will, in general, reduce the overall temperature dependence of our calculated resistivity with the low-temperature ($T \ll T_D$) resistivity showing an approximate saturation behavior.¹²

We emphasize that the screening theory produces excellent qualitative agreement with the existing experimental data and provides a good zeroth-order (q_0, t) scaling description, which is all one should expect from the simple Drude-Boltzmann RPA-screening theory for a strong-coupling (i.e., low carrier density) problem. The question of how valid Boltzmann theory is for understanding 2D metallicity is a difficult question to answer. A serious problem in this respect is the fact that this is the only quantitative theory that exists in the literature for studying 2D metallicity, and therefore its validity can only be judged *a posteriori* through an empirical comparison with the experimental data. (There is simply no competing alternative quantitative theory in this problem, making the discussion of the validity of the RPA-Boltzmann theory somewhat meaningless—we emphasize in this context that the interaction theory of Ref. 21 is not an alternative theory, it is an extension of the RPA theory to incorporate higher-order quantum interaction corrections within necessarily a highly restrictive model; the interaction theory applies only when the temperature correction to conductivity is very small and linear.) We believe that the RPA screening description should be qualitatively well valid in this problem as long as the dominant disorder in the 2D semiconductor systems arises from long-ranged random charged impurity scattering (as is the case here at low carrier densities). This is because RPA is a physically motivated approximation, lead-

ing to the screening of the long-ranged Coulomb scattering potential to a short-ranged screened disorder. The approximation becomes exact only in the limit of high density and high temperature, but the 2D metallicity manifests itself only for finite values of T/T_F (i.e., for T/T_F extremely small ρ does not show strong T dependence!) and as such, RPA should be a reasonable description. We believe that the exactness of RPA in the $r_s \rightarrow 0$ limit has been overemphasized in the literature—RPA remains a qualitatively accurate description of metallic systems even for large values of r_s (particularly at finite T/T_F) as long as there is no quantum phase transition to a non-Fermi-liquid phase. The 2D metal-insulator-transition (2D MIT) being essentially a “high-temperature” phenomenon, RPA, in our opinion, is a reasonable description. The fact that our calculated transport results change little by including local-field corrections (beyond RPA) further reinforces the qualitative validity of RPA to this problem. It should, however, be emphasized that like any other (nonperturbative) uncontrolled approximation (e.g., dynamic mean field theory (DMFT), local-density approximation) the quantitative accuracy of RPA is difficult to ascertain from a purely theoretical viewpoint. One advantage of the RPA-Boltzmann minimal transport model adopted in our work is that transport calculations can be carried out for arbitrary temperatures and carrier densities with concrete comparisons with experimental data. We have carried out one such comparison with a recent experiment²² in this paper (Sec. V), and earlier comparisons exist in the literature.^{14–16,19,23,26,27} The general conclusion one can draw from these comparisons is that the RPA-Boltzmann theory is a reasonably successful *zeroth-order* model for 2D transport properties, providing a qualitative (and intuitively appealing) explanation for the strong 2D metallicity at low carrier densities. As a quantitative theory, however, it is not very successful at lower densities (which is not unexpected), and *ad hoc* theoretical refinements (e.g., assuming a lower effective carrier density or larger effective mass) may be needed for obtaining quantitative agreement with low-density 2D transport data. The systematic quantitative deviation of the leading-order RPA-Boltzmann theory from the experimental data on low-density 2D metallic systems could arise from the large number of effects left out of this zeroth-order theory which take on significance as the carrier density is lowered, such as higher-order (beyond screening) interaction corrections, higher-order impurity scattering effects, possible localization corrections, and various additional scattering processes left out of the theory (e.g., intervalley scattering, bulk impurity scattering, etc.). What is surprising is not that the zeroth-order RPA-Boltzmann theory becomes systematically quantitatively unreliable at lower carrier densities, but the fact that this minimal leading-order theory provides such an excellent qualitative description of the observed 2D metallicity [for example, by explaining the strong variation in $\Delta\rho(T, n)/\rho_0$ in various systems as arising from the difference in the q_0, t values] at all densities and a good quantitative description at higher densities. This is particularly significant in view of the early suggestions made in the literature in the context of the 2D metal-insulator transition physics that the strong 2D metallic behavior must be arising

from some exotic non-Fermi-liquid ground state of the system at low carrier densities. It is now manifestly clear that the apparent 2D metallic behavior arises from standard Fermi-liquid corrections involved in the interplay of interaction and disorder with screened effective disorder arising from the temperature-dependent screening of random charged impurities in the system being the main qualitative source for the strong temperature-dependent 2D resistivity. This high-temperature consequences of the RPA-Boltzmann transport theory for 2D carrier systems are discussed in our companion publication²⁶ with the current manuscript focusing entirely on the low-temperature transport properties.

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APPENDIX

The carrier resistivity ρ in our theory is given by

$$\rho = \frac{m}{ne^2\langle\tau\rangle}, \quad (\text{A1})$$

where m is the carrier effective mass, and the energy averaged transport relaxation time $\langle\tau\rangle$ is given in the Boltzmann theory by

$$\langle\tau\rangle = \frac{\int dE \tau(E) E \left(-\frac{\partial f}{\partial E}\right)}{\int dE E \left(-\frac{\partial f}{\partial E}\right)}, \quad (\text{A2})$$

where $\tau(E)$ is the energy dependent relaxation time, and $f(E)$ is the carrier (Fermi) distribution function. At $T=0$, $f(E) \equiv \theta(E_F - E)$, where E_F is the Fermi energy, and then $\langle\tau\rangle \equiv \tau(E_F)$ giving the familiar result $\sigma \equiv \rho^{-1} = ne^2\tau(E_F)/m$. The Fermi energy for a 2D system is given by $E_F = \pi n \hbar^2 / (g_v m) \equiv k_B T_F$, where a spin degeneracy of 2 has been assumed, and g_v is the valley degeneracy of the 2D system [$g_v=1$ for GaAs; $g_v=2$ for Si (100) MOSFET's].

We calculate the impurity ensemble averaged relaxation time $\tau(E)$ due to elastic disorder scattering in the Born approximation:

$$\frac{1}{\tau(E_k)} = \frac{2\pi}{\hbar} \sum_{\alpha, \mathbf{k}'} \int_{-\infty}^{\infty} dz N_i^{(\alpha)}(z) |u^{(\alpha)}(\mathbf{k} - \mathbf{k}'; z)|^2 \times (1 - \cos \theta_{\mathbf{k}\mathbf{k}'}) \delta(E_k - E_{k'}), \quad (\text{A3})$$

where $E(k) = \hbar^2 k^2 / 2m$ is the 2D carrier energy for 2D wave vector \mathbf{k} ; $\theta_{\mathbf{k}\mathbf{k}'}$ is the scattering angle between carrier scattering wave vectors \mathbf{k} and \mathbf{k}' ; the delta function $\delta(E_k - E_{k'})$ assures energy conservation for elastic scattering due to charged impurities where the screened scattering potential is denoted by $u^{(\alpha)}(\mathbf{q}; z)$ with $\mathbf{q} \equiv \mathbf{k} - \mathbf{k}'$ as the 2D scattering wave vector and z is the quantization or the confinement direction normal to the 2D layer. The quantity $N_i^{(\alpha)}(z)$ in Eq. (A3) denotes the 3D charged impurity density (with the z

dependence reflecting a possible impurity distribution) of the α th kind with α representing the various possible types of impurities which may be present in 2D semiconductor structures. For example, α could denote charged impurities (or interface roughness) located at the interface (e.g., Si-SiO₂ interface for MOSFET's, GaAs-AlGaAs interface for GaAs heterostructures and quantum wells) or impurities in the 2D layer itself or remote charged impurities inside the insulator (which could nevertheless scatter the 2D carriers by virtue of the long-range nature of Coulomb scattering). It is, for example, known that in low-density Si inversion layers the dominant scattering arises from the charged impurities located at the Si-SiO₂ interface. In general, however, the distribution of scattering centers in 2D semiconductor systems is not known, and has to be inferred from a careful comparison between experimental transport data and theoretical calculations assuming various kinds of scatters. Fortunately for our purpose, this lack of precise knowledge of the charged impurity distribution is not a crucial issue since, on the qualitative level of our interest, all of them give rise to strong temperature dependence of the resistivity provided the carrier density is low enough—the temperature dependence is the strongest when the impurities are distributed in the bulk of the 2D layer (bulk impurities) and goes down as the impurities are located further (remote impurities) from the layer inside the insulator. In our calculation presented in this paper, we typically assumes only one kind of scatters parametrized by a single impurity density to keep the number of parameters a minimum—this impurity density essentially sets the overall scale of resistivity in our results. We emphasize that we can obtain good qualitative agreement with almost all the existing 2D MIT experimental data by choosing three different kinds of charged impurities (i.e., interface, remote, and bulk) parametrized by a few reasonable parameters, but we do not see much point in this data fitting-type endeavor.

The screened impurity potential $u^{(\alpha)}(\mathbf{q}; z) \equiv u^{(\alpha)}(q; z)$ is given by

$$u^{(\alpha)}(q; z) \equiv [\epsilon(q)]^{-1} V_{\text{imp}}^{(\alpha)}(q; z), \quad (\text{A4})$$

where $V_{\text{imp}}^{(\alpha)}$ is the bare potential due to a charged impurity and $\epsilon(q)$ is the carrier dielectric function screening the impurity potential. The bare potential is given by

$$V_{\text{imp}}^{(\alpha)}(q; z) = \frac{2\pi Z^{(\alpha)} e^2}{\bar{\kappa} q} F_{\text{imp}}^{(\alpha)}(q; z), \quad (\text{A5})$$

where $Z^{(\alpha)}$ is the impurity charge strength, $\bar{\kappa}$ is the background (static) lattice dielectric constant, and $F_{\text{imp}}^{(\alpha)}$ is a form factor determined by the location of the impurity and the subband wave function $\psi(z)$ defining the 2D confinement. (We do not show the explicit form of the form-factor $F_{\text{imp}}^{(\alpha)}$ here except to note that it reduces to $F_{\text{imp}} = e^{-qd}$ for a strictly 2D layer, where $|\psi(z)|^2 = \delta(z)$, with d being the separation of the impurity from the 2D layer—for $d=0$, i.e., when the impurity is in the layer, $F_{\text{imp}} = 1$ in this pure 2D limit as one would expect.)

The finite wave-vector dielectric screening function is written in the RPA as

$$\epsilon(q) = 1 - v(q)\Pi(q, T), \quad (\text{A6})$$

where $v(q) = v_{2D}(q)f(q)$ is the effective bare electron-electron (Coulomb) interaction in the system with $v_{2D}(q) = 2\pi e^2/(\bar{\kappa}q)$ being the 2D Fourier transform of the usual 3D Coulomb potential, $e^2/(\bar{\kappa}r)$, and $f(q)$ being the Coulomb form factor arising from the subband wave functions $\psi(z)$:

$$f(q) = \frac{1}{2} \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz' |\psi(z)|^2 |\psi(z')|^2 \left[\left(\frac{\kappa_s + \kappa_i}{\kappa_s} \right) e^{-q|z-z'|} + \left(\frac{\kappa_s - \kappa_i}{\kappa_s} \right) e^{-q|z+z'|} \right]. \quad (\text{A7})$$

The second term in Eq. (A7) arises from the image charge effect due to $\kappa_i \neq \kappa_s$, where κ_i and κ_s are the lattice dielectric constants of the insulator and the semiconductor, respectively, [with $\bar{\kappa} = (\kappa_i + \kappa_s)/2$]. We note that in the strict 2D limit, when $|\psi(z)|^2 = \delta(z)$, $f(q) = 1$.

The 2D irreducible finite-temperature (and finite wave vector) polarizability function $\Pi(q; T)$ is given by the noninteracting polarizability (the irreducible ‘‘bubble’’) function within RPA:

$$\Pi(q, T) = \frac{\beta}{4} \int_0^{\infty} d\mu' \frac{\Pi(q; T=0, \mu')}{\cosh^2 \frac{\beta}{2} (\mu - \mu')}, \quad (\text{A8})$$

where $\beta \equiv (k_B T)^{-1}$. In Eq. (A8) $\Pi(q; T=0, E_F)$ is the zero-temperature noninteracting static polarizability given by

$$\Pi(q; T=0, E_F) = N_F \left[1 - \sqrt{1 - \left(\frac{2k_F}{q} \right)^2} \theta(q - 2k_F) \right], \quad (\text{A9})$$

where $N_F = g_v m / \pi$ is the density of states at Fermi energy, and $k_F = (2\pi n / g_v)^{1/2}$ is the 2D Fermi wave vector. The chemical potential μ in Eq. (A8) at finite temperature T is given by

$$\mu = \frac{1}{\beta} \ln[-1 + \exp(\beta E_F)]. \quad (\text{A10})$$

We note that the integration in Eq. (A8) is over the dummy variable μ' which is unrelated to the real Fermi energy E_F of

the system. For going beyond RPA one would rewrite the noninteracting polarizability function $\Pi(q, T)$ to a model interacting polarizability function $\Pi_{\text{int}}(q, T)$ which is written as

$$\Pi_{\text{int}}(q, T) = \frac{\Pi(q, T)}{1 - v(q)G(q, T)\Pi(q, T)}, \quad (\text{A11})$$

where Π is the noninteracting polarizability function described above and $G(q, T)$ is a suitable local-field correction which approximately incorporates correction effects neglected in RPA.

It is now straightforward to see that under the conditions of strict 2D approximation, no remote impurity scattering, only one kind of impurity scattering (i.e., only one value of Z_i and N_i characterizing the impurity scattering strength), and no local-field corrections the calculated resistivity $\rho(T, n)$ of the system expressed as the dimensionless quantity ρ/ρ_0 where $\rho_0 \equiv \rho(T=0)$ depends only on the variables $q_0 \equiv q_{TF}/2k_F$ [with the 2D Tomas-Fermi wave vector $q_{TF} = 2g_v m e^2 / (\bar{\kappa} \hbar^2)$] and $t \equiv T/T_F$, where

$$q_0 \propto g_v^{3/2} \frac{m}{\bar{\kappa}} n^{-1/2}, \quad (\text{A12a})$$

$$t \propto T(g_v m) n^{-1}. \quad (\text{A12b})$$

For our fully realistic calculations (as well as for the experimental system), however, this scaling relation, i.e., an exclusive (q_0, t) dependence of resistivity, is violated due to the quasi-2D nature of the system [i.e., $|\psi(z)|^2 \neq \delta(z)$]; the presence of the insulator (i.e., $\kappa_s \neq \kappa_i$); various types of impurity distributions in the 2D layer, the interface, and in the insulator; local-field corrections, etc. We note that our calculation assumes one subband occupancy, i.e., only the ground 2D subband $\psi(z)$ is considered in our work. At higher temperatures (and lower densities) other (excited) subbands may get occupied by carriers in which case one would have to carry out a multisubband transport calculation including intersubband scattering processes. Such a multisubband generalization of the Drude-Boltzmann formalism given above is straightforward, but the actual calculation of $\rho(T)$ becomes extremely complicated in this situation, and has only been attempted recently in one special case by us²⁵ where we considered intersubband scattering between spin-split subbands in the valance band of *p*-GaAs 2D hole systems.

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